Phosphonic acid, bis(1-methylethyl) ester 1809-20-7 | DTXSID7061988

1809-20-7	D1X2ID7061888

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 193 °C

Global applicability domain: Inside

Local applicability domain index: 7.28e-01

Confidence level: 7.57e-01

Nearest Neighbors from the Training Set

Image not found

Diethyl methanephosphonate

Measured: 194 Predicted: 193

Image not found

Diethyl ethylphosphonate

Measured: 198 Predicted: 196

Image not found

Phosphonic acid, vinyl-, diethyl

ester

Measured: 202 Predicted: 205

Image not found

Triethyl phosphite Measured: 158 Predicted: 168

Image not found

Triethyl phosphate Measured: 216 Predicted: 211